

Supplementary material

Targeting the Class A Carbapenemase GES-5 via Virtual Screening

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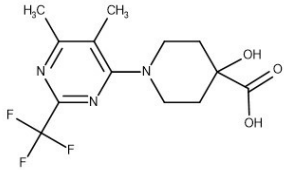
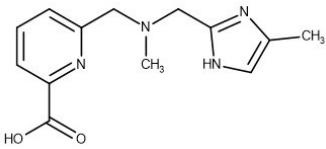
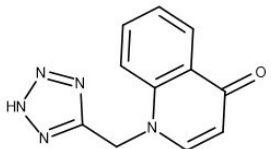
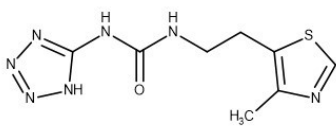
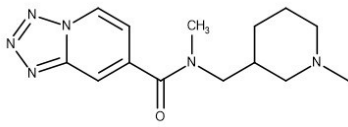
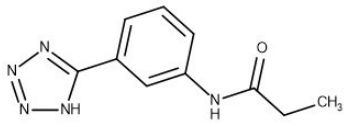
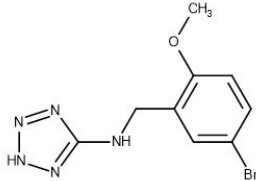
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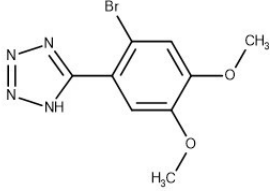
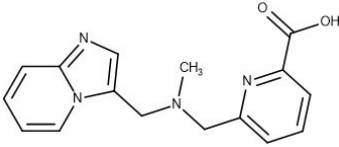
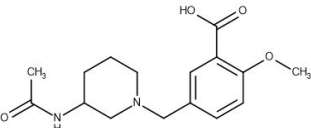
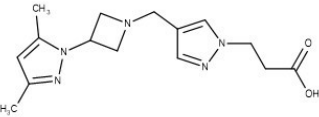
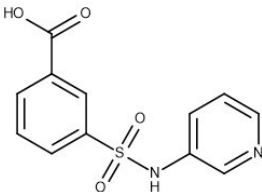
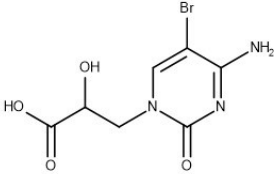
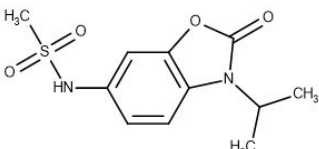
Table S 1: Data collection and refinement statistics.

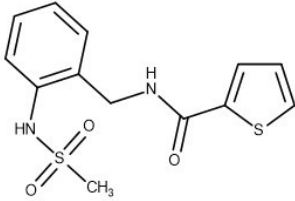
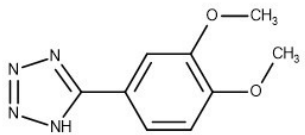
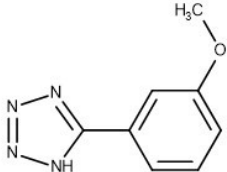
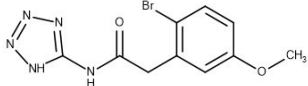
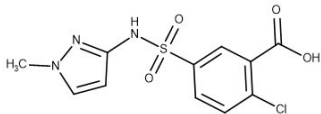
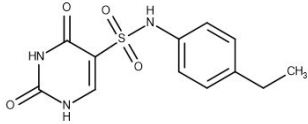
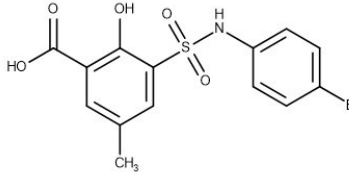
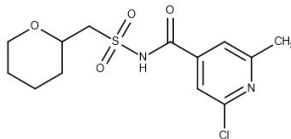
	GES-5
PDB code	6TS9
Wavelength	0.97624
Resolution range	55.33 - 1.55 (1.58 - 1.55)
Space group	P 21 21 21
Unit cell	76.3 80.36 87.85 90 90 90
Unique reflections	78894 (7770)
Multiplicity	6.0 (5.7)
Completeness (%)	99.94 (99.96)
Mean I/sigma(I)	18.96 (2.69)
Wilson B-factor	20.08
R-merge	0.04645 (0.5643)
CC1/2	1 (0.876)
Reflections used in refinement	78892 (7770)
Reflections used for R-free	3915 (394)
R-work	0.1795 (0.2364)
R-free	0.2037 (0.2740)
CC(work)	0.958 (0.835)
CC(free)	0.926 (0.808)
Number of non-hydrogen atoms	4829
macromolecules	4271
ligands	16
solvent	542
Protein residues	537
RMS(bonds)	0.014
RMS(angles)	1.94
Ramachandran favored (%)	97.94
Ramachandran allowed (%)	1.88
Ramachandran outliers (%)	0.19
Rotamer outliers (%)	4.09
Clashscore	7.27
Average B-factor	24.44
macromolecules	22.99
ligands	34.49
solvent	35.57

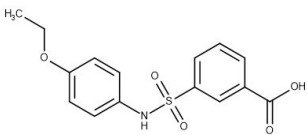
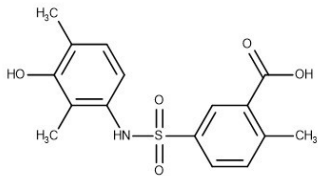
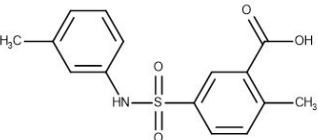
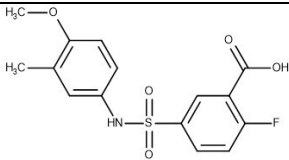
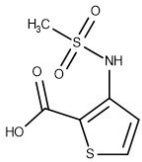
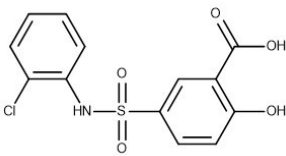
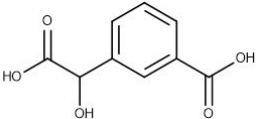
Data for the highest-resolution shell are shown in parentheses.

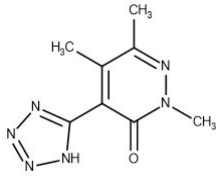
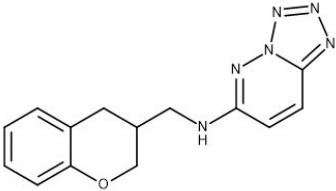
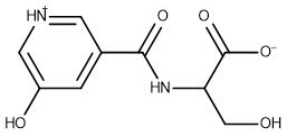
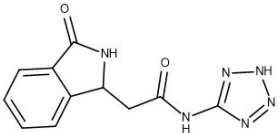
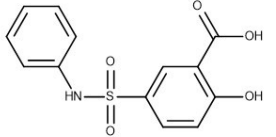
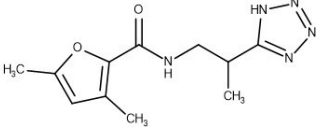
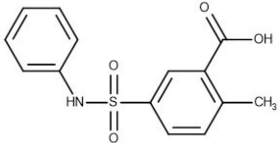
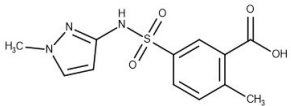
Table S 2: Compound codes, chemical structures and inhibition data for purchased compounds.

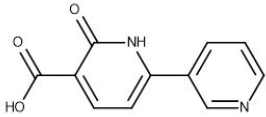
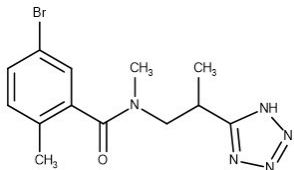
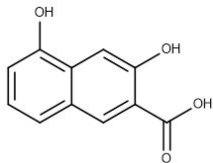
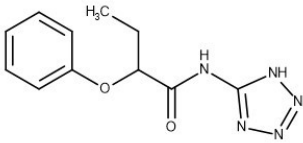
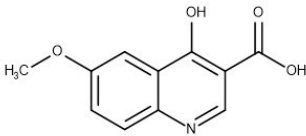
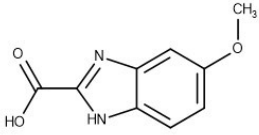
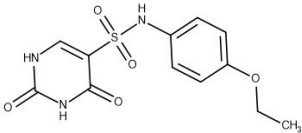
Code	Structure	MolPort ID	MW	% inhibition at [1mM] vs GES-5	% inhibition at [1mM] vs KPC-2
1		MolPort-020- 216-167	319.284	19%	<i>n.d.</i>
2		MolPort-030- 047-117	260.297	21%	26%
3		MolPort-007- 988-798	227.227	18%	<i>n.d.</i>
4		MolPort-005- 142-722	253.28	23%	19%
5		MolPort-020- 210-470	302.382	27%	<i>n.d.</i>
6		MolPort-002- 129-311	217.232	33%	30%
7		MolPort-000- 864-739	284.117	21%	19%

8		MolPort-002-104-350	285.101	IC ₅₀ 1.74	IC ₅₀ 2.31
9		MolPort-035-370-005	296.33	16%	<i>n.d.</i>
10		MolPort-035-383-766	306.362	19%	19%
11		MolPort-030-060-088	303.366	<i>Not tested because of solubility issues</i>	
12		MolPort-002-307-735	278.28	IC ₅₀ 1.98	IC ₅₀ 2.71
13		MolPort-003-884-547	278.062	IC ₅₀ 1.58	IC ₅₀ 1.86
14		MolPort-007-617-735	270.3	10%	<i>n.d.</i>

15		MolPort-009-318-942	310.39	16%	<i>n.d.</i>
16		MolPort-001-005-590	206.205	<i>n.d.</i>	<i>n.d.</i>
17		MolPort-002-467-448	176.179	28%	17%
18		MolPort-027-913-957	312.127	21%	18%
19		MolPort-009-422-837	315.73	34%	20%
20		MolPort-003-130-164	295.31	26%	24%
21		MolPort-009-350-762	386.22	32%	24%
22		MolPort-035-847-366	332.8	18%	21%

23		MolPort-002-305-656	321.35	29%	44%
24		MolPort-009-556-594	335.37	32%	31%
25		MolPort-002-462-443	305.35	23%	28%
26		MolPort-020-063-552	339.34	30%	30%
27		MolPort-009-460-556	221.25	19%	29%
28		MolPort-002-363-286	327.74	29%	40%
29		MolPort-021-943-905	196.158	19%	22%

30		MolPort-005-311-448	206.209	Not tested because of solubility issues	
31		MolPort-009-435-655	282.307	Not tested because of solubility issues	
32		MolPort-000-768-609	226.188	21%	14%
33		MolPort-027-846-104	258.241	20%	20%
34		MolPort-000-644-251	293.29	Not tested because of solubility issues	
35		MolPort-030-031-849	249.274	24%	27%
36		MolPort-005-178-145	291.32	21%	n.d.
37		MolPort-005-705-646	295.31	23%	n.d.

38		MolPort-006-756-424	216.196	Not tested because of solubility issues	
39		MolPort-035-750-522	338.209	21%	n.d.
40		MolPort-001-790-951	204.181	23%	n.d.
41		MolPort-001-544-523	247.258	33%	24%
42		MolPort-000-004-269	219.196	Not tested because of solubility issues	
43		MolPort-019-878-939	192.174	IC ₅₀ 1.29	IC ₅₀ 1.88
44		MolPort-003-130-166	311.31	23%	n.d.

n.d: not determined